

On Faces of the set of Quantum Channels

Raphael Loewy

Department of Mathematics

Technion – Israel Institute of Technology

loewy@tx.technion.ac.il

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Abstract

A linear map L from $\mathbb{C}^{n \times n}$ into $\mathbb{C}^{n \times n}$ is called a quantum channel if it is completely positive and trace preserving. The set \mathcal{L}_n of all such quantum channels is known to be a compact convex set. While the extreme points of \mathcal{L}_n can be characterized, not much is known about the structure of its higher dimensional faces. Using the so called Choi matrix $Z(L)$ associated with the quantum channel L , we compute the maximum dimension of a proper face of \mathcal{L}_n , and in addition the possible dimensions of faces generated by L when $\text{rank } Z(L) = 2$.

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0 Introduction

Let $\mathbb{C}^{n \times n}$, \mathcal{H}_n and $PSD_n \subset \mathcal{H}_n$ denote, respectively, the sets of all $n \times n$ complex matrices, complex hermitian matrices and positive semidefinite matrices. A *pure state* is a positive semidefinite matrix of rank 1 and trace 1. Let \mathcal{P}_n denote the set of pure states in \mathcal{H}_n . Let $[m] = \{1, 2, \dots, m\}$ for any positive integer m .

A linear operator $L : \mathbb{C}^{n \times n} \rightarrow \mathbb{C}^{n \times n}$ is called *completely positive* if

$$L(X) = \sum_{i=1}^k A_i X A_i^*, \quad A_i \in \mathbb{C}^{n \times n}, \quad i \in [k]. \quad (0.1)$$

A completely positive operator which is also trace preserving is called *quantum channel*. It is known and straightforward to see that if L is given by (0.1) then it is a quantum channel if and only if

$$\sum_{i=1}^k A_i^* A_i = I_n, \quad (0.2)$$

where I_n denotes the identity matrix of order n .

Let \mathcal{L}_n denote the set of all quantum channels defined on $\mathbb{C}^{n \times n}$. Then \mathcal{L}_n is a compact convex set, and it is the purpose of this paper to consider its face structure. The 0-dimensional faces are the extreme points of \mathcal{L}_n , and they are of fundamental importance, thus attracting significant attention, cf. [Ch], [FL], [RSW], [Ru]. One characterization, due to Choi [Ch], is given in terms of the matrices A_i appearing in (0.1). Another way to decide whether $L \in \mathcal{L}_n$ is an extreme point is to use the so called *Choi matrix* $Z(L)$ associated with L .

For $i, j \in [n]$ let $E_{ij} \in \mathbb{C}^{n \times n}$ denote the matrix with 1 in the ij position and 0's elsewhere. Then

$$Z(L) = [L(E_{ij})]_{i,j=1}^n. \quad (0.3)$$

It is well known that a linear operator $L : \mathbb{C}^{n \times n} \rightarrow \mathbb{C}^{n \times n}$ is completely positive if and only if $Z(L)$ is positive semidefinite. Moreover, letting $A = Z(L) = [A_{ij}]_{i,j=1}^n$ with $A_{ij} \in \mathbb{C}^{n \times n}$ for $i, j \in [n]$, then a completely positive L is a quantum channel if and only if the trace conditions $\text{tr} A_{ij} = \delta_{ij}$ also hold for $i, j \in [n]$.

Friedland and Loewy [FL] gave a necessary and sufficient condition for $L \in \mathcal{L}_n$ to be an extreme point in terms of the null space of $Z(L)$. It is pointed out in [Ch, Remark 6], see also Ruskai, Szarek Werner [RSW] and Ruskai [Ru], that if $L \in \mathcal{L}_n$ is an extreme point, then $\text{rank} Z(L) \leq n$.

It seems that higher dimensional faces of \mathcal{L}_n have not attracted much attention, although they are of interest as well as the extreme points. Our purpose here is to consider some of those faces. The paper is organized as follows: In Section 1 we give some additional notation and some preliminary results. In Section 2 we consider faces generated by matrices $Z(L)$ such that $\text{rank} Z(L) = 2$ and determine their possible dimensions. In Section 3 we show the maximum dimension of a proper face of \mathcal{L}_n is $n^4 - 3n^2 + 1$. The concept of *face* is basic in convex set theory, and the reader is referred to [Ro] for related information.

1 Preliminaries

We first introduce some additional notation. Given $A \in \mathbb{C}^{n \times n}$ and $\alpha, \beta \subset [n]$ let $A[\alpha|\beta]$ be the submatrix of A based on rows in α and columns in β , and let $A[\alpha] = A[\alpha|\alpha]$. Also, given any matrix A denote by $A^{(j)}$ its j -th column. Given positive integers r and s let \mathcal{J}_{rs} be the all ones matrix of order $r \times s$, and let $\mathcal{J}_r = \mathcal{J}_{rr}$. We use the standard inner product, denoted by $\langle \cdot, \cdot \rangle$.

Let

$$\mathcal{C}_n = \{A = [A_{ij}]_{i,j=1}^n \in \text{PSD}_{n^2}, A_{ij} \in \mathbb{C}^{n \times n}, \text{tr} A_{ij} = \delta_{ij}, i, j \in [n]\}. \quad (1.1)$$

Then, \mathcal{C}_n is a compact convex set in the real vector space \mathcal{H}_{n^2} of dimension $n^4 - n^2$, and the map from \mathcal{L}_n to \mathcal{C}_n defined by $L \rightarrow Z(L)$ is an isomorphism (see [FL]). Given any $A \in \mathcal{C}_n$, denote by $\mathcal{F}(A)$ the face of \mathcal{C}_n generated by A .

The smallest affine subspace of \mathcal{H}_{n^2} containing \mathcal{C}_n is

$$\mathcal{W}_n = \{A = [A_{ij}]_{i,j=1}^n \in \mathcal{H}_{n^2}, A_{ij} \in \mathbb{C}^{n \times n}, \text{tr} A = \delta_{ij}, i, j \in [n]\}. \quad (1.2)$$

We note that the (relative) interior of \mathcal{C}_n consists of all positive definite matrices in \mathcal{C}_n . Indeed, every positive definite matrix in \mathcal{C}_n is in its (relative) interior. Since $\frac{1}{n}I_{n^2} \in \mathcal{C}_n$, it follows that if $A \in \mathcal{C}_n$ is singular then for any $\varepsilon > 0$ $(1 + \varepsilon)A - \frac{\varepsilon}{n}I_{n^2} \in \mathcal{W}_n$ and has a negative eigenvalue. Hence A belongs to the (relative) boundary of \mathcal{C}_n .

The following observation characterizes the rank 1 matrices in \mathcal{C}_n .

Observation 1.1 Let $x = (x_1^t, x_2^t, \dots, x_n^t)^t \in \mathbb{C}^{n^2}$, where $x_i \in \mathbb{C}^n$ for all $i \in [n]$. Then $xx^* \in \mathcal{C}_n$ if and only if $\{x_i\}_{i \in [n]}$ forms an orthonormal basis of \mathbb{C}^n with respect to the standard inner product.

Proof: It is clear that $\{x_i\}_{i \in [n]}$ forms an arthonormal basis with respect to the standard inner product if and only if the trace conditions in (1.1) are satisfied by xx^* . \square

The next lemma is useful when considering faces of \mathcal{C}_n .

Lemma 1.1 Let $A \in \mathcal{C}_n$ and $B \in \mathcal{F}(A)$. Then,

(a) $\ker A \subset \ker B$,

(b) If B belongs to the (relative) boundary of $\mathcal{F}(A)$, $\text{rank} B < \text{rank} A$.

Proof: Since A belongs to the (relative) interior of $\mathcal{F}(A)$ there exist $0 < \alpha \leq 1$ and $C \in \mathcal{C}_n$ such that $A = \alpha B + (1 - \alpha)C$. Then (a) follows because if $AX = 0$ then $x^*Ax = \alpha x^*Bx + (1 - \alpha)x^*Cx = 0$, implying $Bx = 0$.

To prove (b) assume B belongs to the (relative) boundary of $\mathcal{F}(A)$. For any $\varepsilon \in \mathbb{R}$, $(1 + \varepsilon)B - \varepsilon A \in \mathcal{W}_n$. Suppose that $\text{rank} B = \text{rank} A$. Then there exists $\varepsilon > 0$ sufficiently small such that $(1 + \varepsilon)B - \varepsilon A$ is positive semidefinite, so belongs to \mathcal{C}_n .

This can be seen, for example, by the known result that A and B can be simultaneously diagonalized by a congruence, and with the positive elements on both diagonal matrices appearing in the same locations. It follows that there exist $C \in \mathcal{C}_n$ and $0 < \alpha < 1$ such that $B = \alpha A + (1 - \alpha)C$, so B belongs to the (relative) interior of \mathcal{C}_n , a contradiction. \square

As a consequence of the previous lemma we get a simple geometric proof of the following known result.

Corollary 1.1 Every matrix in \mathcal{C}_n is a convex combination of at most n^2 extreme points.

Proof: Let $A \in \mathcal{C}_n$ and consider $\mathcal{F}(A)$. It is well known that every extreme point of $\mathcal{F}(A)$ is also an extreme point of \mathcal{C}_n . Take such an extreme point, say B , and continue the line segment from A to B until it meets the (relative) boundary of $\mathcal{F}(A)$ at a point C . This is possible because \mathcal{C}_n is compact. Then A is a convex combination of B and C , and by Lemma 1.1 $\text{rank} C < \text{rank} A$. Repeat the process with C . As $\text{rank} A \leq n^2$ the process consists of at most n^2 steps, completing the proof. \square

2 The dimension of $\mathcal{F}(L)$ when $\text{rank} Z(L) = 2$

Our goal here is to find out the possible dimensions that $F(L)$ can attain when $\text{rank} Z(L) = 2$.

Theorem 2.1 *Let $L \in \mathcal{L}_n$ with $\text{rank} Z(L) = 2$. Then*

- (i) $\dim \mathcal{F}(L)$ is 0 or 2 if $n = 2$,
- (ii) $\dim \mathcal{F}(L)$ is 0 or 1 or 2 if $n \geq 3$.

Proof: It follows from Theorems 1 and 12 of [FL] that $L(\mathcal{P}_m)$ contains a pure state, and since we can apply (independently) unitary similarities in the domain and range, we can assume without loss of generality that $L(E_{11}) = E_{11}$. Also, for convenience, we write $A = Z(L)$.

(i) Suppose first that $n = 2$. Then, as $L \in \mathcal{L}_2$, we have (cf. (6.1) of [FL])

$$A = \begin{bmatrix} 1 & 0 & 0 & y \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1-c & s \\ \bar{y} & 0 & \bar{s} & c \end{bmatrix},$$

and by assumption $\text{rank}(A) = 2$. As $A \in \text{PSD}_4$, we have $0 \leq c \leq 1$. If $c = 1$ then $s = 0$ and $|y| < 1$. For every $B \in \mathcal{F}(A)$ $\ker B \supset \ker A$ by Lemma 1.1, hence $e_2, e_3 \in \ker B$. Therefore $\mathcal{F}(A)$ consists of all matrices

$$\begin{bmatrix} 1 & 0 & 0 & z \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \bar{z} & 0 & 0 & 1 \end{bmatrix}$$

with $z \in \mathbb{C}$, $|z| \leq 1$, so $\dim \mathcal{F}(A) = 2$.

Assume now that $0 \leq c < 1$. In this case the first and third columns of A form a basis for its column space, and we must have

$$\begin{bmatrix} y \\ 0 \\ s \\ c \end{bmatrix} = y \begin{bmatrix} 1 \\ 0 \\ 0 \\ \bar{y} \end{bmatrix} + \frac{s}{1-c} \begin{bmatrix} 0 \\ 0 \\ 1-c \\ \bar{s} \end{bmatrix}. \quad (2.1)$$

Note the entries of A have to satisfy

$$(1 - c)(c - |y|^2) = |s|^2. \quad (2.2)$$

We will show now that if $B \in \mathcal{F}(A)$ then $B = A$, implying that $\dim \mathcal{F}(A) = 0$. It follows from (2.1) that e_2 and $e_4 - ye_1 - \frac{s}{1-c}e_3$ form a basis of $\ker A$, and hence belong to $\ker B$ for $B \in \mathcal{F}(A)$. There exists $0 \leq c_1 \leq 1$ such that $b_{33} = 1 - c_1$. Hence $b_{14} = y$, $b_{34} = \frac{s(1-c_1)}{1-c}$, $b_{43} = \frac{\bar{s}(1-c_1)}{1-c}$ and $b_{44} = yb_{41} + \frac{s}{1-c}b_{43} = |y|^2 + \frac{|s|^2(1-c_1)}{(1-c)^2}$.

As $b_{33} + b_{44} = 1$ we get

$$1 - c_1 + |y|^2 + \frac{|s|^2(1 - c_1)}{(1 - c)^2} = 1.$$

Using (2.2), we get

$$(1 - c)^2(|y|^2 - c_1) + (1 - c)(c - |y|^2)(1 - c_1) = 0,$$

so

$$(c - c_1)(1 - |y|^2) = 0,$$

and as $c < 1$ implies $|y| < 1$, we conclude that $c = c_1$, $b_{33} = a_{33}$, $b_{34} = a_{34}$ and $b_{44} = a_{44}$. Hence $B = A$.

(ii) Suppose now that $n \geq 3$. The proof is by induction on n , although the induction hypothesis will not be used in all subcases to follow.

Recall that $L(E_{11}) = E_{11}$, so rows and columns of A indexed by $2, 3, \dots, n$ are 0. This implies, as $L \in \mathcal{L}_n$, $a_{1,n+1} = 0$. We distinguish several cases.

(iia) Suppose that there exists a positive integer i , $1 \neq i < n^2$, $i \equiv 1 \pmod{n}$ such that $a_{ii} > 0$. Without loss of generality we may assume

$$a_{n+1,n+1} > 0. \quad (2.3)$$

Since $\text{rank} A = 2 = \text{rank} A[\{1, n+1\}]$, we must have by a Schur complement argument

$$\begin{aligned} A[\{n+2, n+3, \dots, n^2\}] &= \\ A[\{n+2, n+3, \dots, n^2\}|\{1, n+1\}] \begin{bmatrix} 1 & 0 \\ 0 & a_{n+1,n+1}^{-1} \end{bmatrix} A[\{1, n+1\}|\{n+2, n+3, \dots, n^2\}]. \end{aligned} \quad (2.4)$$

In particular, (2.4) implies

$$a_{n+j,n+j} = |a_{1,n+j}|^2 + \frac{|a_{n+1,n+j}|^2}{a_{n+1,n+1}}, \quad j = 2, 3, \dots, n. \quad (2.5)$$

We must also have

$$\sum_{j=n+1}^{2n} a_{jj} = 1. \quad (2.6)$$

We intend to show that A is an extreme point in this case. For that purpose, assume that

$$A = \alpha C + (1 - \alpha)D, \quad C, D \in \mathcal{C}_n, \quad 0 < \alpha < 1.$$

By Lemma 1.1 $\ker C \supset \ker A$ and $\ker D \supset \ker A$. The standard unit vectors e_2, e_3, \dots, e_n belong to $\ker A$, so also to $\ker C, \ker D$. This means that rows and columns of C , as well as of D , indexed by $2, 3, \dots, n$ are 0. Also, trace conditions imposed by $C, D \in \mathcal{C}_n$ imply

$$c_{11} = d_{11} = 1 \text{ and } c_{1i} = d_{1i} = c_{i1} = d_{i1} = 0 \text{ for } 1 \neq i < n^2, \quad i \equiv 1 \pmod{n}.$$

The column vectors $A^{(1)}, A^{(n+1)} \in \mathbb{C}^{n^2}$ form a basis for the column space of A . So it is straightforward that

$$A^{(j)} = a_{1j}A^{(1)} + \frac{a_{n+1,j}}{a_{n+1,n+1}}A^{(n+1)}, \quad n+2 \leq j \leq n^2, \quad (2.7)$$

implying that $e_j - a_{1j}e_1 - \frac{a_{n+1,j}}{a_{n+1,n+1}}e_{n+1} \in \ker A \subset \ker C, \ker D$.

Hence, for $n+2 \leq j \leq n^2$,

$$C^{(j)} = a_{1j}C^{(1)} + \frac{a_{n+1,j}}{a_{n+1,n+1}}C^{(n+1)}; \quad D^{(j)} = a_{1j}D^{(1)} + \frac{a_{n+1,j}}{a_{n+1,n+1}}D^{(n+1)}. \quad (2.8)$$

This implies

$$c_{1j} = a_{1j}c_{11} + \frac{a_{n+1,j}}{a_{n+1,n+1}}c_{n+1,1} = 1 \cdot a_{1j} + 0 \cdot \frac{a_{n+1,j}}{a_{n+1,n+1}} = a_{1j}, \quad (2.9)$$

and similarly

$$d_{1j} = a_{1j}. \quad (2.10)$$

Therefore,

$$c_{j1} = d_{j1} = a_{j1}. \quad (2.11)$$

Using $c_{n+1,1} = d_{n+1,1} = 0$, we obtain from (2.8)

$$c_{n+1,j} = \frac{a_{n+1,j}c_{n+1,n+1}}{a_{n+1,n+1}} ; \quad d_{n+1,j} = \frac{a_{n+1,j}d_{n+1,n+1}}{a_{n+1,n+1}} ; \quad (2.12)$$

$$c_{j,n+1} = \bar{c}_{n+1,j} ; \quad d_{j,n+1} = \bar{d}_{n+1,j}.$$

We let $n+2 \leq j \leq 2n$ and apply (2.7) and (2.8), using also (2.9), (2.10), (2.11) and (2.12), to get

$$c_{jj} = |a_{ij}|^2 + \frac{|a_{n+1,j}|^2 c_{n+1,n+1}}{a_{n+1,n+1}^2}, \quad (2.13)$$

$$d_{jj} = |a_{ij}|^2 + \frac{|a_{n+1,j}|^2 d_{n+1,n+1}}{a_{n+1,n+1}^2}. \quad (2.14)$$

Substituting (2.5) into (2.6) yields

$$a_{n+1,n+1} + \sum_{j=n+2}^{2n} \left(|a_{ij}|^2 + \frac{|a_{n+1,j}|^2}{a_{n+1,n+1}} \right) = 1,$$

so

$$a_{n+1,n+1}^2 + a_{n+1,n+1} \sum_{j=n+2}^{2n} |a_{ij}|^2 + \sum_{j=n+2}^{2n} |a_{n+1,j}|^2 = a_{n+1,n+1}. \quad (2.15)$$

Since $C \in \mathcal{C}_n$ we have $\sum_{j=n+1}^{2n} c_{jj} = 1$, so (2.13) implies

$$a_{n+1,n+1}^2 c_{n+1,n+1} + a_{n+1,n+1}^2 \sum_{j=n+2}^{2n} |a_{ij}|^2 + c_{n+1,n+1} \sum_{j=n+2}^{2n} |a_{n+1,j}|^2 = a_{n+1,n+1}^2. \quad (2.16)$$

It follows from (2.15) and (2.16) that

$$a_{n+1,n+1}^2 (c_{n+1,n+1} - a_{n+1,n+1}) + (c_{n+1,n+1} - a_{n+1,n+1}) \sum_{j=n+2}^{2n} |a_{n+1,j}|^2 = 0,$$

and by (2.3) we may conclude that

$$c_{n+1,n+1} = a_{n+1,n+1}, \quad (2.17)$$

which upon substitution into (2.12) yields

$$c_{n+1,j} = a_{n+1,j} \text{ and } c_{j,n+1} = a_{j,n+1} \text{ for } n+2 \leq j \leq n^2, \quad (2.18)$$

and together with (2.9) and (2.11) we conclude

$$C[\{1, n+1\}|\{n+2, n+3, \dots, n^2\}] = A[\{1, n+1\}|\{n+2, n+3, \dots, n^2\}], \quad (2.19)$$

and

$$C[\{n+2, n+3, \dots, n^2\}|\{1, n+1\}] = A[\{n+2, n+3, \dots, n^2\}|\{1, n+1\}]. \quad (2.20)$$

The analogue of (2.4) holds for C , and by (2.18), (2.19) and $C[\{1, n+1\}] = A[\{1, n+1\}]$ we conclude

$$C[\{n+2, n+3, \dots, n^2\}] = A[\{n+2, n+3, \dots, n^2\}],$$

leading finally to $C = A$, which in turn implies $D = A$. Hence A is an extreme point in this case.

(iib) We can assume now that

$$a_{n+1,n+1} = a_{2n+1,2n+1} = \dots = a_{(n-1)n+1,(n-1)n+1} = 0,$$

and this implies that rows and columns of A indexed by $2, 3, \dots, n, n+1, 2n+1, \dots, (n-1)n+1$ are 0. Define

$$S = [n^2] \setminus \{1, 2, \dots, n, n+1, 2n+1, \dots, (n-1)n+1\}, \quad S_1 = S \cup \{1\}, \quad (2.21)$$

and $B = A[S]$, $v = A[\{1\}|S]$, $\tilde{B} = A[S_1]$. So

$$\tilde{B} = \begin{bmatrix} a_{11} & v \\ v^* & B \end{bmatrix} \in \mathbb{C}^{n^2-2n+2 \times n^2-2n+2}.$$

Note that $B \in \mathcal{C}_{n-1}$, and its rank is 1 or 2. We distinguish 2 subcases.

(iib1) Suppose that B is an extreme point of \mathcal{C}_{n-1} . We will show that $\dim \mathcal{F}(A)$ must be 0 or 2. If A is an extreme point we are done, so assume this is not the case.

Then there exist F, G in \mathcal{C}_n , $F \neq G$, such that $A = \frac{1}{2}(F + G)$.

Then, for $\Delta := A - F = (\delta_{ij}) \in \mathbb{C}^{n^2 \times n^2}$ we have

$$G = A + \Delta, \quad F = A - \Delta, \quad B = \frac{1}{2}(F[S] + G[S]).$$

Clearly, $F[S], G[S] \in \mathcal{C}_{n-1}$, and as B is an extreme point of \mathcal{C}_{n-1} (by assumption), we must have

$$B = F[S] = G[S] \Rightarrow \Delta[S] = 0. \quad (2.22)$$

Let $w = \Delta[\{1\}|S]$. Then for $0 \leq t \leq 1$, we have

$$(A + t\Delta)[S_1] = \begin{bmatrix} a_{11} & v + tw \\ v^* + tw^* & B \end{bmatrix}.$$

Moreover, since $\Delta \neq 0$ while $\Delta[S] = 0$ and $\delta_{11} = 0$ (as $b_{11} = g_{11} = a_{11} = 1$), it follows that $w \neq 0$. By symmetry we may assume

$$\delta_{1,n+2} \neq 0. \quad (2.23)$$

For $-1 \leq t \leq 1$, $A + t\Delta \in \mathcal{F}(A)$, so its rank is at most 2. Therefore, for $n+3 \leq j \leq n^2$, $j \not\equiv 1 \pmod{n}$,

$$\det \begin{bmatrix} 1 & a_{1,n+2} + t\delta_{1,n+2} & a_{1j} + t\delta_{1j} \\ \bar{a}_{1,n+2} + t\bar{\delta}_{1,n+2} & a_{n+2,n+2} & a_{n+2,j} \\ \bar{a}_{1j} + t\bar{\delta}_{1j} & \bar{a}_{n+2,j} & a_{jj} \end{bmatrix} = 0,$$

and as $t \in [-1, 1]$ is arbitrary, the coefficient of t^2 in the expansion must vanish, so

$$-|\delta_{1,n+2}|^2 a_{jj} - |\delta_{1j}|^2 a_{n+2,n+2} + \delta_{1,n+2} \bar{\delta}_{1j} a_{n+2,j} + \bar{\delta}_{1,n+2} \delta_{1j} \bar{a}_{n+2,j} = 0. \quad (2.24)$$

Hence, for the positive semidefinite matrix $A[\{n+2, j\}]$ and for $y := \begin{bmatrix} \delta_{1j} \\ -\delta_{1,n+2} \end{bmatrix}$, we get from (2.24),

$$y^* A[\{n+2, j\}] y = 0,$$

or, equivalently,

$$A[\{n+2, j\}] y = 0. \quad (2.25)$$

Since A is positive semidefinite it follows from (2.25) that

$$A^{(j)} = \frac{\delta_{1j}}{\delta_{1,n+2}} A^{(n+2)} \text{ for } n+3 \leq j \leq n^2, \ j \not\equiv 1 \pmod{n}. \quad (2.26)$$

Note also that we must have $\det A[\{1, n+2\}] > 0$, or else $A^{(1)}$ and $A^{(n+2)}$ are linearly dependent, leading to $\text{rank} A = 1$, a contradiction. In particular, we have $a_{n+2,n+2} > 0$ and $|a_{1,n+2}|^2 < a_{n+2,n+2}$.

The previous discussion shows that $A^{(1)}$ and $A^{(n+2)}$ are linearly independent, and the following is a basis for $\ker A$, and thus included in the kernel of any matrix in $\mathcal{F}(A)$:

$$\{e_2, e_3, \dots, e_n, e_{n+1}, e_{2n+1}, \dots, e_{(n-1)n+1}, \delta_{1,n+2}e_j - \delta_{1j}e_{n+2}, \ j \in S \setminus \{n+2\}\}.$$

Hence, given any $X = (x_{ij}) \in \mathcal{F}(A)$ we have $x_{11} = 1$, $X[[n^2] \setminus \{1\}] = A[[n^2] \setminus \{1\}]$ and

$$X[\{1\}|S] = [x_{1,n+2}, \frac{\delta_{1,n+3}}{\delta_{1,n+2}}x_{1,n+2}, \frac{\delta_{1,n+4}}{\delta_{1,n+2}}x_{1,n+2}, \dots, \frac{\delta_{1,n^2}}{\delta_{1,n+2}}x_{1,n+2}],$$

with $|x_{1,n+2}|^2 < a_{n+2,n+2}$. This shows that $\dim \mathcal{F}(A) = 2$.

(iib2) It remains to consider the case that $B = A[S]$ is not an extreme point of \mathcal{C}_{n-1} . This implies immediately that $\text{rank} B = 2$, so there exist distinct $k, l \in S$ such that $A^{(k)}, A^{(l)}$ are linearly independent, and $\alpha_k, \alpha_l \in \mathbb{C}$ such that

$$A^{(1)} = \alpha_k A^{(k)} + \alpha_l A^{(l)}. \quad (2.27)$$

Define a linear map $\varphi : \mathcal{H}_{n^2} \rightarrow \mathcal{H}_{(n-1)^2}$ by $\varphi(H) = H[S]$. We claim that φ is 1-1 on $\mathcal{F}(A)$. Indeed, suppose that $X, Y \in \mathcal{F}(A)$ with $\varphi(X) = \varphi(Y)$. It follows from (2.27) and Lemma 1.1 that $e_1 - \alpha_k e_k - \alpha_l e_l \in \ker A \subset \ker X, \ker Y$. Hence $X^{(1)} = \alpha_k X^{(k)} + \alpha_l X^{(l)}$ and $Y^{(1)} = \alpha_k Y^{(k)} + \alpha_l Y^{(l)}$, and since $X[S] = Y[S]$ and $x_{11} = y_{11} = 1$ it follows that $X = Y$.

By the induction hypothesis $\dim \mathcal{F}(B) \leq 2$ in \mathcal{C}_{n-1} (actually we know it is positive by assumption that B is not extreme), and therefore in this subcase we can also conclude that $\dim \mathcal{F}(A) \leq 2$, and combining with the previous subcases, the same inequality holds always when $\text{rank} A = 2$.

In the rest of the proof we show that all possible dimensions of $\mathcal{F}(L)$ are attained. This has already been demonstrated when $n = 2$ in the proof of (i), so assume now $n \geq 3$.

The following example shows that case (ia) can occur.

Let $y = [e_1^t, 0^t, 0^t, \dots, 0^t]^t \in \mathbb{C}^{n^2}$ and $z = [0^t, e_1^t, e_2^t, \dots, e_{n-1}^t]^t \in \mathbb{C}^{n^2}$, and let $A = yy^* + zz^*$. Clearly $A \in \mathcal{C}_n$ and $\text{rank} A = 2$. Note that $\text{rank} A[n+1, n+2, \dots, n^2] = 1$.

Next, we demonstrate that both possibilities that are discussed in (ib1) can occur. Start with $B \in \mathcal{C}_{n-1}$ which is an extreme point and with $\text{rank} B = 2$, and we may assume without loss of generality that $b_{11} > 0$. To get an extreme point $A \in \mathcal{C}_n$ with $A[S] = B$ (where S is defined by (2.21)) let the rows and columns of A indexed by $2, 3, \dots, n, n+1, 2n+1, (n-1)n+1$ be 0. Let $A[\{1\}|S] = \frac{1}{\sqrt{a_{n+2, n+2}}} A[\{n+2\}|S] = [b_{11}, b_{12}, \dots, b_{1, (n-1)^2}]^t$, $a_{11} = 1$. It follows that $A^{(1)} = \frac{1}{\sqrt{a_{n+2, n+2}}} A^{(n+2)}$, so $e_1 - \frac{1}{\sqrt{a_{n+2, n+2}}} e_{n+2} \in \ker A$, hence to the kernel of every matrix in $\mathcal{F}(A)$. This and the extremality of B in \mathcal{C}_{n-1} imply that A is an extreme point of \mathcal{C}_n .

The second possibility arising in (ib1) is realized by starting with a rank 1 extreme point $B \in \mathcal{C}_{n-1}$ (we may assume again $b_{11} > 0$). We define (hermitian) A by letting $A[S] = B$, $a_{11} = 1$, $A[\{1\}|S] = 0$, and all rows and columns of A indexed by $2, 3, \dots, n, n+1, 2n+1, \dots, (n-1)n+1$ be 0. Then it is straightforward to see that $A \in \mathcal{C}_n$, and $\dim \mathcal{F}(A) = 2$.

Finally, we show that for any $n \geq 3$ there exists $A \in \mathcal{C}_n$ satisfying (ib2) and such that $\dim \mathcal{F}(A) = 1$. We start with $n = 3$ and define

$$P = \begin{bmatrix} 1 & \frac{9}{4\sqrt{6}} & \frac{3}{2\sqrt{6}} \\ \frac{9}{4\sqrt{6}} & 1 & \frac{1}{4} \\ \frac{3}{2\sqrt{6}} & \frac{1}{4} & 1 \end{bmatrix}. \quad (2.28)$$

Then $P \in PSD_3$ and $Pq = 0$, where $q = [1, -\frac{2}{\sqrt{6}}, -\frac{1}{\sqrt{6}}]^t$. Let

$$A_3 = \begin{bmatrix} E_{11} & \frac{9}{4\sqrt{6}} E_{12} & \frac{3}{2\sqrt{6}} E_{13} \\ \frac{9}{4\sqrt{6}} E_{21} & E_{22} & \frac{1}{4} E_{23} \\ \frac{3}{2\sqrt{6}} E_{31} & \frac{1}{4} E_{32} & E_{33} \end{bmatrix} \in \mathbb{C}^{9 \times 9}. \quad (2.29)$$

Then $A_3[\{159\}] = P$, so $A_3 \in \mathcal{C}_3$ and $\text{rank} A_3 = 2$. Note also $L(E_{11}) = E_{11}$ (where $A_3 = Z(L)$). We claim that $\dim \mathcal{F}(A_3) = 1$. The vectors $e_2, e_3, e_4, e_6, e_7, e_8$ and $e_1 - \frac{2}{\sqrt{6}} e_5 - \frac{1}{\sqrt{6}} e_9$ form a basis of $\ker A_3$, thus belonging to the kernel of every matrix in $\mathcal{F}(A_3)$. Let X be any extreme point of $\mathcal{F}(A_3)$, then, necessarily, $\text{rank} X = 1$. Also, $X^{(j)} = 0$ for $j = 2, 3, 4, 6, 7, 8$.

There exist $x_1, x_2, x_3 \in \mathbb{C}$ such that

$$X[\{1, 5, 9\}] = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} [\bar{x}_1 \ \bar{x}_2 \ \bar{x}_3],$$

and we must also have $|x_i| = 1$, $i = 1, 2, 3$. Without loss of generality assume $x_1 = 1$, and let $x_2 = e^{-i\theta}$, $x_3 = e^{-i\varphi}$, where $\theta, \varphi \in \mathbb{R}$. The condition $e_1 - \frac{2}{\sqrt{6}}e_5 - \frac{1}{\sqrt{6}}e_9 \in \ker X$ leads to the equation (over \mathbb{C})

$$2e^{i\theta} + e^{i\varphi} = \sqrt{6},$$

or, equivalently, two equations (over \mathbb{R})

$$2\cos\theta + \cos\varphi = \sqrt{6}, \text{ and } 2\sin\theta + \sin\varphi = 0. \quad (2.30)$$

Since $\sqrt{6} > 2$ it follows from (2.30) that $\cos\theta, \cos\varphi > 0$, so $\theta, \varphi \in (-\frac{\pi}{2}, \frac{\pi}{2})$. Moreover, $\sin\theta$ and $\sin\varphi$ must have opposite signs. We have

$$1 - 4\sin^2\theta = 1 - \sin^2\varphi = \cos^2\varphi = 6 - 4\sqrt{6}\cos\theta + 4\cos^2\theta,$$

so

$$4\sqrt{6}\cos\theta = 9,$$

implying

$$\cos\theta = \frac{9}{4\sqrt{6}} \text{ and } \sin\theta = \pm \frac{1}{4}\sqrt{\frac{5}{2}}. \quad (2.31)$$

Hence

$$\cos\varphi = \sqrt{6} - \frac{9}{2\sqrt{6}} = \frac{3}{2\sqrt{6}} \text{ and } \sin\varphi = \mp \frac{1}{2}\sqrt{\frac{5}{2}}. \quad (2.32)$$

Thus, (2.30) has 2 solutions, (θ_1, φ_1) with $0 < \theta_1 < \frac{\pi}{2}$, $-\frac{\pi}{2} < \varphi_1 < 0$, and (θ_2, φ_2) with $-\frac{\pi}{2} < \theta_2 < 0$, $0 < \varphi_2 < \frac{\pi}{2}$, corresponding to the expressions obtained in (2.31) and (2.32), including the signs in the appropriate order. This shows that $\mathcal{F}(A_3)$ has 2 extreme points, X and X_1 . Here we write only their nontrivial part, namely $X[\{159\}]$ and $X_1[\{159\}]$.

$$X[\{159\}] = \begin{bmatrix} 1 & e^{i\theta_1} & e^{i\varphi_1} \\ e^{-i\theta_1} & 1 & e^{i(\varphi_1-\theta_1)} \\ e^{-i\varphi_1} & e^{i(\theta_1-\varphi_1)} & 1 \end{bmatrix}, \quad X_1[\{159\}] = \begin{bmatrix} 1 & e^{i\theta_2} & e^{i\varphi_2} \\ e^{-i\theta_2} & 1 & e^{i(\varphi_2-\theta_2)} \\ e^{-i\varphi_2} & e^{i(\theta_2-\varphi_2)} & 1 \end{bmatrix},$$

so

$$X[\{159\}] = \begin{bmatrix} 1 & \frac{9}{4\sqrt{6}} + \frac{\sqrt{5}}{4\sqrt{2}}i & \frac{3}{2\sqrt{6}} - \frac{\sqrt{5}}{2\sqrt{2}}i \\ \frac{9}{4\sqrt{6}} - \frac{\sqrt{5}}{4\sqrt{2}}i & 1 & \frac{1}{4} - \frac{\sqrt{15}}{4}i \\ \frac{3}{2\sqrt{6}} + \frac{\sqrt{5}}{2\sqrt{2}}i & \frac{1}{4} + \frac{\sqrt{15}}{4}i & 1 \end{bmatrix} = \bar{X}_1[\{159\}].$$

Note that $A = \frac{1}{2}(X + X_1)$.

The construction of $A \in \mathcal{C}_n$ satisfying (iib2) and $\dim \mathcal{F}(A) = 1$ is based on the construction of A_3 in (2.29). Let $n \geq 3$ and $A^{[n]} = [A_{ij}]_{i,j=1,2,\dots,n} \in \mathbb{C}^{n^2 \times n^2}$, where $A_{ij} = E_{ij} \in \mathbb{C}^{n \times n}$ for $i, j \in [n-2]$; $A_{i,n-1} = A_{n-1,i}^t = \frac{9}{4\sqrt{6}}E_{i,n-1} \in \mathbb{C}^{n \times n}$ and $A_{in} = A_{ni}^t = \frac{3}{2\sqrt{6}}E_{in} \in \mathbb{C}^{n \times n}$ for $i \in [n-2]$; $A_{ii} = E_{ii} \in \mathbb{C}^{n \times n}$ for $i = n-1, n$; $A_{n-1,n} = A_{n,n-1}^t = \frac{1}{4}E_{n-1,n} \in \mathbb{C}^{n \times n}$.

Note that $A^{[3]} = A_3$, and clearly $A^{[n]} \in \mathcal{C}_n$. Moreover, for the corresponding quantum channel L (so that $A^{[n]} = Z(L)$) we have $L(E_{11}) = E_{11}$. Furthermore, whenever $n \geq 4$, for the set S defined in (2.21), we have $A^{[n]}[S] = A^{[n-1]}$, so $A^{[n-1]}$ is embedded as a principal submatrix in $A^{[n]}$.

Let $S_2 = \{(n+1)i+1, i=0, 1, 2, \dots, n-1\}$. Then the only nonzero rows (and columns) of $A^{[n]}$ are those indexed by elements in S_2 , and we have

$$A^{[n]}[S_2] = \begin{bmatrix} J_{n-2} & \frac{9}{4\sqrt{6}}J_{n-2,1} & \frac{3}{2\sqrt{6}}J_{n-2,1} \\ \frac{9}{4\sqrt{6}}J_{1,n-2} & 1 & \frac{1}{4} \\ \frac{3}{2\sqrt{6}}J_{1,n-2} & \frac{1}{4} & 1 \end{bmatrix}.$$

The latter matrix is congruent to the direct sum of P , defined in (2.28), and the 0 matrix of order $n-3$, hence $\text{rank } A^{[n]} = 2$. Therefore any extreme matrix X in $\mathcal{F}(A^{[n]})$ must have $\text{rank } 1$, and its kernel must contain $\ker A^{[n]}$. Write $X = xx^*$, $x = (x_j) \in \mathbb{C}^{n^2}$. Then $x_j = 0$ for $j \notin S_2$, and $|x_j| = 1$ for $j \in S_2$. We may normalize so that $x_1 = 1$, and $\ker X$ forces $x_j = 1$ for any $j \in S_2$, except for $j = (n+1)(n-2)+1$ and $j = (n+1)(n-1)+1 = n^2$. The proof proceeds now as in the case of $n = 3$. \square

3 Proper faces of \mathcal{L}_n of maximum dimension

Our main goal here is to compute the maximum dimension of a proper face of \mathcal{L}_n , or equivalently \mathcal{C}_n . We start with the following lemma.

Lemma 3.1 *Let $A \in \mathcal{C}_n$ with $r = \text{rank} A$, and assume $r \leq n^2 - 2$. Then $\mathcal{F}(A)$ is strictly contained in a proper face of \mathcal{C}_n generated by a matrix of rank $r + 1$.*

Proof: There exists $x = [x_1^t, x_2^t, \dots, x_n^t]^t \in \mathbb{C}^{n^2} \neq 0$, $x \in \ker A$, where $x_i = (x_i^{(j)}) \in \mathbb{C}^n$, $i \in [n]$. Therefore, there exist $1 \leq i, j \leq n$ such that $x_i^{(j)} \neq 0$. Let σ be a permutation of $[n]$ such that $\sigma(i) = j$, and let $u = [e_{\sigma(1)}^t, e_{\sigma(2)}^t, \dots, e_{\sigma(i-1)}^t, e^{i\theta} e_{\sigma(i)}^t, \dots, e_{\sigma(n)}^t]^t \in \mathbb{C}^{n^2}$, with $\theta \in \mathbb{R}$ to be determined. By Observation (1.1) $uu^* \in \mathcal{C}_n$, and θ can be chosen so that $\langle u, x \rangle \neq 0$. Let $A_1 = \frac{1}{2}(A + uu^*)$. Then $A_1 \in \mathcal{C}_n$ with $\text{rank} A_1 = r + 1 < n^2$, and $\mathcal{F}(A_1)$ is a proper face of \mathcal{C}_n , strictly containing $\mathcal{F}(A)$. \square

It follows from the lemma that to compute the maximum dimension of a proper face of \mathcal{C}_n it suffices to consider matrices in \mathcal{C}_n of rank $n^2 - 1$.

Observation 3.1 *Suppose that $L \in \mathcal{L}_n$ with $A = Z[L] = [A_{ij}]_{i,j=1}^n$, and suppose that $z = [z_1^t, z_2^t, \dots, z_n^t]^t \in \ker A$, with $z_i \in \mathbb{C}^n$, $i \in [n]$. Let $U \in \mathbb{C}^{n \times n}$ be any unitary matrix. Then $A_1 = [UA_{ij}U^*]_{i,j=1}^n = Z[L_1]$ for some $L_1 \in \mathcal{L}_n$, and $[(Uz_1)^t, (Uz_2)^t, \dots, (Uz_n)^t]^t \in \ker A_1$.*

Proof: Since $A \in \mathcal{C}_n$ so is A_1 , and the rest is clear. \square

Theorem 3.1 *Let $n \geq 2$ be an integer. Then the maximum dimension of a proper face of \mathcal{L}_n (equivalently \mathcal{C}_n) is $n^4 - 3n^2 + 1$.*

Proof: We consider \mathcal{C}_n , and by Lemma 3.1 it suffices to consider faces generated by matrices in \mathcal{C}_n of rank $n^2 - 1$. We start with $n = 2$, which has to be dealt with separately.

$n = 2$ Suppose that $A \in \mathcal{C}_2$ with $\text{rank} A = 3$, and let $z = [v^t, w^t]^t$, $v, w \in \mathbb{C}^2$ be a nonzero vector in $\ker A$ (it is uniquely determined up to a scalar multiple). We may assume without loss of generality that $v \neq 0$, and using scaling and Observation 3.1 we may assume $v = e_1$.

Suppose first that v, w are linearly dependent, so $w = \alpha e_1$ for some $\alpha \in \mathbb{C}$. Then $Az = 0$ yields the following system:

$$\begin{aligned} a_{11} &= -\alpha a_{13}, \\ \bar{a}_{12} &= -\alpha a_{23}, \\ \bar{a}_{13} &= -\alpha a_{33}, \\ \bar{a}_{14} &= -\alpha \bar{a}_{34}, \end{aligned}$$

which together with the trace conditions imposed by $A \in \mathcal{C}_2$ yield

$$A = \begin{bmatrix} |\alpha|^2 a_{33} & -\bar{\alpha} \bar{a}_{23} & -\bar{\alpha} a_{33} & -\bar{\alpha} a_{34} \\ -\alpha a_{23} & 1 - |\alpha|^2 a_{33} & a_{23} & \bar{\alpha} a_{33} \\ -\alpha a_{33} & \bar{a}_{23} & a_{33} & a_{34} \\ -\alpha \bar{a}_{34} & \alpha a_{33} & \bar{a}_{34} & 1 - a_{33} \end{bmatrix}.$$

As a_{33} , a_{23} and a_{34} are free variables (subject to $A \in PSD_4$), we see that $\dim \mathcal{F}(A) = 5$.

We may assume now that v, w are linearly independent, so let $w = [\alpha, \beta]^t \in \mathbb{C}^2$, with $\beta \neq 0$. Then $Az = 0$ yields the following system:

$$\begin{aligned} a_{11} + \alpha a_{13} + \beta a_{14} &= 0, \\ \bar{a}_{12} + \alpha a_{23} - \beta a_{13} &= 0, \\ \bar{a}_{13} + \alpha a_{33} + \beta a_{34} &= 0, \\ \bar{a}_{14} + \alpha \bar{a}_{34} + \beta(1 - a_{33}) &= 0. \end{aligned}$$

Note that we must have $0 < a_{11} < 1$ and $0 < a_{33} < 1$, or else $\text{rank} A = 2$. It follows from the system that

$$\begin{aligned} a_{13} &= -\bar{\alpha} a_{33} - \bar{\beta} \bar{a}_{34}, \\ a_{14} &= -\bar{\alpha} a_{34} - \bar{\beta}(1 - a_{33}), \\ a_{12} &= -\bar{\alpha} \bar{a}_{23} + \bar{\beta}(-\alpha a_{33} - \beta a_{34}) = -\bar{\alpha} \bar{a}_{23} - \alpha \bar{\beta} a_{33} - |\beta|^2 a_{34}, \\ a_{11} &= -\alpha(-\bar{\alpha} a_{33} - \bar{\beta} \bar{a}_{34}) - \beta(-\bar{\alpha} a_{34} - \bar{\beta} + \bar{\beta} a_{33}) = \\ &= (|\alpha|^2 - |\beta|^2) a_{33} + \alpha \bar{\beta} \bar{a}_{34} + \bar{\alpha} \beta a_{34} + |\beta|^2, \end{aligned}$$

which together with $\gamma := |\alpha|^2 - |\beta|^2$ and the trace conditions yield

$$A = \begin{bmatrix} \gamma a_{33} + 2\text{Re}(\alpha \bar{\beta} \bar{a}_{34}) + |\beta|^2 & -\bar{\alpha} \bar{a}_{23} - \alpha \bar{\beta} a_{33} - |\beta|^2 a_{34} & -\bar{\alpha} a_{33} - \bar{\beta} \bar{a}_{34} & -\bar{\alpha} a_{34} - \bar{\beta}(1 - a_{33}) \\ -\alpha a_{23} - \bar{\alpha} \beta a_{33} - |\beta|^2 \bar{a}_{34} & 1 - \gamma a_{33} - 2\text{Re}(\alpha \bar{\beta} \bar{a}_{34}) - |\beta|^2 & a_{23} & \bar{\alpha} a_{33} + \bar{\beta} \bar{a}_{34} \\ -\alpha a_{33} - \beta a_{34} & \bar{a}_{23} & a_{33} & a_{34} \\ -\alpha \bar{a}_{34} - \beta(1 - a_{33}) & \alpha a_{33} + \beta a_{34} & \bar{a}_{34} & 1 - a_{33} \end{bmatrix}.$$

As a_{33} , a_{23} and a_{34} are free variables (subject to $A \in PSD_4$), we get $\dim \mathcal{F}(A) = 5$.

$n \geq 3$ Suppose that $A \in \mathcal{C}_n$ such that $\text{rank} A = n^2 - 1$. Then, there exists $x = (x_i) \in \mathbb{C}^{n^2}$ (unique up to scalar multiples) such that $Ax = 0$. We may

assume without loss of generality, using scaling and Observation 3.1, that $x_{n^2} = 1$ and $x_{n^2-1} \neq 0$.

Write $A = [A_{ij}]_{i,j=1}^n$, with $A_{ij} \in \mathbb{C}^{n \times n}$. By assumption, A has to satisfy the linear equations $\text{tr} A_{ij} = \delta_{ij}$ for $i, j \in [n]$, and $Ax = 0$. We will show that $\dim \mathcal{F}(A) = n^4 - 3n^2 + 1$ by using these equations to express certain entries of A in terms of the other entries. More precisely, the following discussion will show that the following are not free variables: $(i)a_{i,n^2}$, $i \in [n^2]$ and $i \not\equiv 0 \pmod{n}$; a_{kn,n^2-1} , $k \in [n-1]$; a_{n^2,n^2} ; For $1 \leq i \leq j \leq n$, the first entry on the main diagonal of A_{ij} .

We use first the trace conditions. For $1 \leq i \leq j \leq n$ we use $\text{tr} A_{ij} = \delta_{ij}$ to express the first entry on its main diagonal in terms of its successors. So, for example, $a_{11} = 1 - \sum_{i=2}^n a_{ii}$, $a_{1,n+1} = -\sum_{i=2}^n a_{i,n+i}$, etc.

Next we consider the kernel condition, namely the n^2 homogeneous, linear equations $(Ax)_i = 0$, $i \in [n^2]$. We consider them sequentially, and as we will see, eliminating at each step exactly one of the remaining non-free variables that is, either a_{i,n^2} or a_{i,n^2-1} for a suitable i . We consider these equations in the natural order.

Suppose that $i \in [n^2 - 1]$. When $i \not\equiv 0 \pmod{n}$ we use $(Ax)_i = 0$ to eliminate a_{i,n^2} . Let $f_i^{(n^2)}$ be the (linear) expression obtained when writing a_{i,n^2} in terms of free variables. When $i \equiv 0 \pmod{n}$, $i < n$, we use $(Ax)_i = 0$ to eliminate a_{i,n^2-1} . Let $f_i^{(n^2-1)}$ be the (linear) expression obtained when writing a_{i,n^2-1} in terms of free variables (this is possible since $x_{n^2-1} \neq 0$).

For example,

$$f_1^{(n^2)} = - \sum_{j=1}^{n^2-1} a_{1j} x_j = - \sum_{\substack{j=1 \\ j \not\equiv 1 \pmod{n}}}^{n^2-1} a_{1j} x_j - 1x_1 + \sum_{i=2}^n \sum_{k=0}^{n-1} a_{i,i+kn} x_{1+kn},$$

$$f_n^{(n^2-1)} = -\frac{1}{x_{n^2-1}} \cdot \sum_{\substack{j=1 \\ j \neq n^2-1}}^{n^2} a_{nj} x_j = -\frac{1}{x_{n^2-1}} \left(\sum_{j=1}^{n-1} \bar{a}_{jn} x_j + \sum_{\substack{j=n \\ j \neq n^2-1}}^{n^2} a_{nj} x_j \right).$$

We finally get to the last equation, that is, $(Ax)_{n^2} = 0$, and show it will determine a_{n^2,n^2} . Note that a_{n^2,n^2} appears also in the equation $(Ax)_{(n-1)n+1} = 0$, which has already been discussed. Hence it appears in $f_{n^2-n+1}^{(n^2)}$, and so it

appears in the summand $a_{n^2, n^2-n+1}x_{n^2-n+1} = \bar{f}_{n^2-n+1}^{(n^2)}x_{n^2-n+1}$ in $(Ax)_{n^2} = 0$. So a_{n^2, n^2} appears twice in the last equation. Recall that a_{n^2, n^2} is real, and we will prove that the last equation determines a_{n^2, n^2} in a well defined way, completing the counting of the non-free variables.

Consider now the appearance of each free variable in the last equation. We distinguish several cases, each dealing with a free variable. As A is hermitian, we have $a_{ji} = \bar{a}_{ij}$, so free variables appear on the main diagonal or above. The first two cases deal with main diagonal entries.

- (I) Consider a main diagonal entry a_{ii} , where $i \not\equiv 1, n(\text{mod } n)$. Write $i = qn + r$, where $0 \leq q \leq n-1$ and $2 \leq r \leq n-1$. Then a_{ii} appears in $(Ax)_i = 0$ and $(Ax)_{i-r+1} = 0$, hence in $f_i^{(n^2)}$ and $f_{i-r+1}^{n^2}$ with coefficients $-x_i$ and x_{i-r+1} , respectively. Therefore, the summands in the left hand side of $(Ax)_{n^2} = 0$ containing a_{ii} are $-\overline{a_{ii}x_i}x_i + \overline{a_{ii}x_{i-r+1}}x_{i-r+1}a_{ii}(|x_{i-r+1}|^2 - |x_i|^2) \in \mathbb{R}$.
- (II) Consider a main diagonal entry a_{ii} , where $i \equiv 0(\text{mod } n)$, $i \leq n^2 - 1$. Then a_{ii} appears in $(Ax)_i = 0$ and $(Ax)_{i-n+1} = 0$. The latter yields that a_{ii} appears in $f_{i-n+1}^{(n^2)}$ with coefficient x_{i-n+1} . The former yields that a_{ii} appears in $f_i^{(n^2-1)}$ with coefficient $-\frac{x_i}{x_{n^2-1}}$. Hence a_{ii} appears in $(Ax)_{n^2-1} = 0$, and so it appears in $f_{n^2-1}^{(n^2)}$ with coefficient $\frac{|x_i|^2}{\bar{x}_{n^2-1}}$. Hence, the summands in the left hand side of $(Ax)_{n^2} = 0$ containing a_{ii} are $a_{ii}(|x_{i-n+1}|^2 + |x_i|^2) \in \mathbb{R}$.
- (III) Consider a_{ij} (a free variable) that does not appear on either of the main diagonal, last row, last column of the block A_{kl} containing it. Then a_{ij} appears in $f_i^{(n^2)}$ with coefficient $-x_j$ and $a_{ji} = \bar{a}_{ij}$ appears in $f_j^{(n^2)}$ with coefficient $-x_i$. Hence, the summands in the left hand side of $(Ax)_{n^2} = 0$ containing a_{ij}, a_{ji} are $-\overline{a_{ij}x_j}x_i - \overline{a_{ji}x_i}x_j = -2\text{Re}(a_{ij}x_j\bar{x}_i) \in \mathbb{R}$.
- (IV) Consider a_{ij} (a free variable) that appears in the last column of the block A_{kl} containing it, but not on its main diagonal. So $i \not\equiv 0(\text{mod } n)$, $j \equiv 0(\text{mod } n)$. Then a_{ij} appears in $f_i^{(n^2)}$ with coefficient $-x_j$, and $a_{ji} = \bar{a}_{ij}$ appears in $f_j^{(n^2-1)}$ with coefficient $-\frac{x_i}{x_{n^2-1}}$. This implies that \bar{a}_{ji} appears in $f_{n^2-1}^{(n^2)}$ with coefficient $\frac{\bar{x}_i x_j}{\bar{x}_{n^2-1}}$. Hence, the summands in the

left hand side of $(Ax)_{n^2} = 0$ containing a_{ij}, a_{ji} are $-\bar{a}_{ij}\bar{x}_j x_i + a_{ji}x_i \bar{x}_j = 0$.

(V) Consider a_{ij} (a free variable) that appears in the last row of the block A_{kl} containing it, but not on its main diagonal. So $i \equiv 0(\text{mod } n)$ and $j \not\equiv 0(\text{mod } n)$. Then a_{ij} appears in $f_i^{(n^2-1)}$ with coefficient $-\frac{x_j}{x_{n^2-1}}$, so $\bar{a}_{ij} = a_{ji}$ appears in $f_{n^2-1}^{(n^2)}$ with coefficient $\frac{\bar{x}_j x_i}{\bar{x}_{n^2-1}}$. Also, $a_{ji} = \bar{a}_{ij}$ appears in $f_j^{(n^2)}$ with coefficient $-x_i$. Hence, the summands in the left hand side of $(Ax)_{n^2} = 0$ containing a_{ij}, a_{ji} are $a_{ij}x_j \bar{x}_i - a_{ij}\bar{x}_i x_j = 0$.

(VI) Consider a free variable a_{i,n^2} , so necessarily $i \equiv 0(\text{mod } n)$ and $i < n^2$. Then a_{i,n^2} appears in $f_i^{(n^2-1)}$ with coefficient $-\frac{1}{x_{n^2-1}}$, so \bar{a}_{i,n^2} appears in $f_{n^2-1}^{(n^2)}$ with coefficient $\frac{x_i}{\bar{x}_{n^2-1}}$. Also, a_{i,n^2} appears as a summand in the expression for a_{i-n+1,n^2-n+1} , and its coefficient in $f_{i-n+1}^{(n^2)}$ is x_{n^2-n+1} . On the other hand $a_{n^2,i} = \bar{a}_{i,n^2}$ appears in the last equation with coefficient x_i , and also in $f_{n^2-n+1}^{(n^2)}$ with coefficient x_{i-n+1} . Hence, the summands in the left hand side of $(Ax)_{n^2} = 0$ containing $a_{i,n^2}, a_{n^2,i}$ are

$$a_{i,n^2}\bar{x}_i + \bar{a}_{i,n^2}\bar{x}_{n^2-n+1}x_{i-n+1} + \bar{a}_{i,n^2}x_i + a_{i,n^2}\bar{x}_{i-n+1}x_{n^2-n+1} \in \mathbb{R}$$

The next two cases deal with a free variable that lies on the main diagonal of the block containing it, but not on the last column of A .

(VII) Consider a free variable a_{ij} , such that $i \not\equiv 0(\text{mod } n)$ and $j \equiv i(\text{mod } n)$ and $j < n^2$. Write $i = qn + r$, where $0 \leq q \leq n-1$ and $1 < r \leq n-1$ (note that we cannot have $r = 1$). Then a_{ij} appears in $f_i^{(n^2)}$ with coefficient $-x_j$, and it also appears as a summand in the expression for $a_{i-r+1,j-r+1}$. Hence it appears in $f_{i-r+1}^{(n^2)}$ with coefficient x_{j-r+1} . Also, $a_{ji} = \bar{a}_{ij}$ appears in $f_j^{(n^2)}$ with coefficient $-x_i$ and in $f_{j-r+1}^{(n^2)}$ with coefficient x_{i-r+1} . Hence, the summands in the left hand side of $(Ax)_{n^2} = 0$ containing a_{ij}, a_{ji} are $-\bar{a}_{ij}\bar{x}_j x_i + \bar{a}_{ij}\bar{x}_{j-r+1}x_{i-r+1} - a_{ij}\bar{x}_i x_j + a_{ij}\bar{x}_{i-r+1}x_{j-r+1} \in \mathbb{R}$.

(VIII) Consider a free variable a_{ij} , such that $i \equiv 0(\text{mod } n)$ and $j \equiv i(\text{mod } n)$ and $j < n^2$. Then a_{ij} appears in $f_i^{(n^2-1)}$ with coefficient $-\frac{x_j}{x_{n^2-1}}$, so $\bar{a}_{ij} = a_{ji}$ appears in $f_{n^2-1}^{(n^2)}$ with coefficient $\frac{\bar{x}_j x_i}{\bar{x}_{n^2-1}}$. Also, a_{ij} is a summand in $a_{i-n+1,j-n+1}$ with coefficient $-x_{j-n+1}$, so it appears in $f_{i-n+1}^{(n^2)}$

with coefficient x_{j-n+1} . In addition, $a_{ji} = \bar{a}_{ij}$ appears in $f_j^{(n^2-1)}$ with coefficient $-\frac{x_i}{x_{n^2-1}}$, so a_{ij} appears in $f_{n^2-1}^{(n^2)}$ with coefficient $\frac{\bar{x}_i x_j}{\bar{x}_{n^2-1}}$. Also, a_{ji} appears in $f_{j-n+1}^{(n^2)}$ with coefficient x_{i-n+1} . Hence, the summands in the left hand side of $(Ax)_{n^2} = 0$ containing a_{ij}, a_{ji} are $a_{ij}x_j\bar{x}_i + \bar{a}_{ij}\bar{x}_{j-n+1}x_{i-n+1} + \bar{a}_{ij}x_i\bar{x}_j + a_{ij}\bar{x}_{i-n+1}x_{j-n+1} \in \mathbb{R}$.

- (IX) Finally we consider the coefficient of a_{n^2, n^2} in the last equation. As a_{n^2, n^2} appears in a summand in the expression for a_{n^2-n+1, n^2-n+1} with coefficient $-x_{n^2-n+1}$, it appears in $f_{n^2-n+1}^{(n^2)}$ with coefficient x_{n^2-n+1} , so the coefficient of a_{n^2, n^2} in the last equation is $|x_{n^2-n+1}|^2 + 1 > 0$. As all other summands in the left hand side of $(Ax)_{n^2} = 0$ are real, as we have shown, it follows that this equation determines a_{n^2, n^2} , completing the proof. \square

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